

CAS SciFinder®

# CAS SCIFINDER DISCOVERY PLATFORM FOR ACADEMICSTM 紹介 セミナー

化学情報協会 情報事業部

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# CAS SciFinder Discovery Platform for Academics の概要

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## CAS SciFinder Discovery Platform for Academicsとは

教育研究機関を対象にした研究活動を総合的にサポートするサービス

CAS SciFinder Discovery Platform for Academics に含まれるサービス

### — CAS SciFinder

文献、化学物質、反応情報、物性、規制情報検索サービス

### — CAS Analytical Methods

分析手法の調査に特化した検索サービス

### — CAS Formulus

製剤・配合情報に特化した検索サービス

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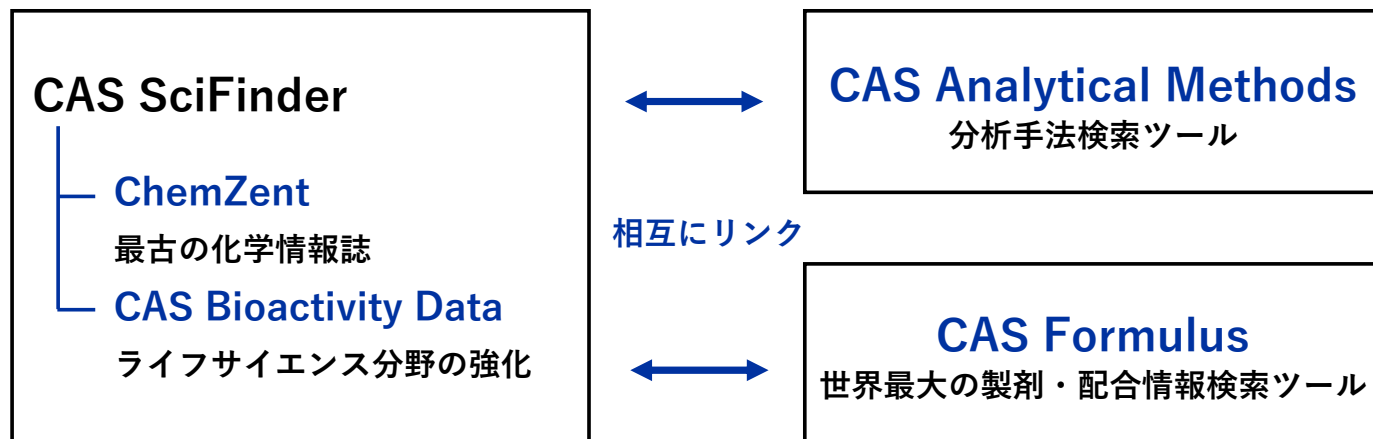
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教育研究機関を対象にした研究活動を総合的にサポートするサービス

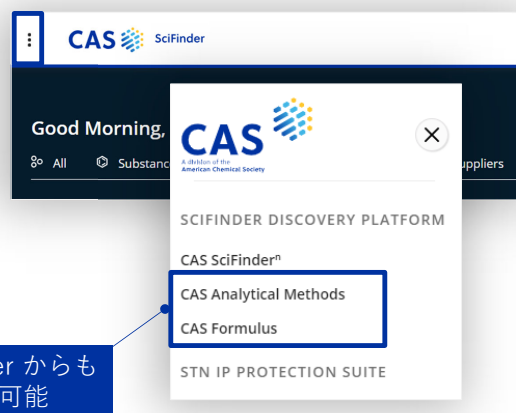
CAS SciFinder Discovery Platform から追加されたコンテンツ (青字)



## アクセス方法

Username (ID)、パスワードはすべて CAS SciFinder と共通

製品名	接続先 URL
CAS SciFinder	<a href="https://scifinder-n.cas.org/">https://scifinder-n.cas.org/</a>
CAS Analytical Methods	<a href="https://methods.cas.org/">https://methods.cas.org/</a>
CAS Formulus	<a href="https://formulus.cas.org/">https://formulus.cas.org/</a>



# CAS SciFinder のライフサイエンスコンテンツ

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## CAS SciFinder のライフサイエンスコンテンツ

### — MEDLINE

生物医学分野の文献データベース (PubMed の情報)  
CAS SciFinder の References で検索できる

### — CAS Sequences

8 億件以上の核酸・タンパク質の配列情報を収録  
3 つのホモロジー検索プログラム (BLAST/CDR/Motif) を登載

### — CAS Bioactivity Data

SAR (構造活性相関)、ADME (吸収、分布、代謝、排泄)、Toxicity (毒性) 情報  
ターゲットやリガンド、疾患を指定した検索

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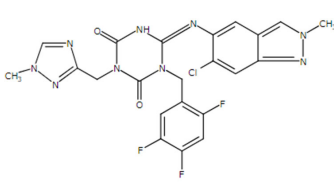
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# CAS Bioactivity Data

物質の生物活性情報と出典文献情報を紐づけて収録

**CAS Registry Number: 264** エントレルビルの物質情報




エントレルビルの構造活性関連データ

Target	Function	Parameter	Value	Disease	Organism	Assay	Source
Replicase polyprotein 1ab	Inhibitor	EC50	0.17 μM	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS
Replicase polyprotein 1ab	Inhibitor	EC50	0.27 μM	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS
Replicase polyprotein 1ab	Inhibitor	EC50	0.22 μM	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS
Replicase polyprotein 1ab	Inhibitor	EC50 ratio	1.59	COVID-19	Severe acute respiratory syndrome coronavirus 2	View Detail	(1) CAS

Novel Investigational Anti-SARS-CoV-2 Agent Ensitrelvir "S-217622": A Broad-Spectrum Antiviral at the Therapeutic Frontline of Coronavirus **出典文献情報**

By: Elsayb, Wafa A.; Abdalla, Mohamed; Rabie, Amgad M. DOI: 10.1021/acsmedchem.3c00581

Later, nirogous heterocyclic antivirals, such as nucleoside-like compounds, oxadiazoles, thiadiazoles, triazoles, quinolines, and isopyridines, topped the therapeutic scene as promising agents of choice for the treatment of the severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) infections and their accompanying ailment, the coronavirus disease 2019 (COVID-19). At the same time, the continuous emergence of new strains of SARS-CoV-2, like the Omicron variant and its multiple sublineages, resulted in a new defiance in the enduring COVID-19 battle. Ensitrelvir (S-217622) is a newly discovered orally active noncovalent nonpeptidic agent with potential strong broad-spectrum anticonviral activities, exhibiting promising nanomolar potencies against the different SARS-CoV-2 variants. S-217622 effectively and nonspecifically hits the main protease (M<sup>pro</sup>) enzyme of a broad scope of coronaviruses. Hence, in the present computational/bio. study, we tried to extend these previous findings to prove the universal activities of this investigational agent against any coronavirus, irres. of its type, through synchronously acting on most of its main unchanged replication enzymes/proteins, including (in addition to the M<sup>pro</sup>), e.g., the highly conserved RNA-dependent RNA polymerase (RdRp) and 3'-5' exoribonuclease (ExoN). Biochem. evaluation proved, using the in vitro anti-RdRp/ExoN bioassay, that S-217622 can potently inhibit the replication of coronaviruses, including the new virulent strains of SARS-CoV-2, with extremely minute in vitro anti-RdRp and anti-ExoN (both half-maximal effective concentration (EC<sub>50</sub>) values of 0.17 and 0.27 μM, resp., transcending the anti-COVID-19 drug molnupiravir. The preliminary in silico results greatly supported these biochem. results, proposing that the S-217622 mol. strongly and stably binds the key catalytic pockets of the SARS-CoV-2 RdRps and ExoNs principal active sites predictably via the nucleoside analogism mode of anti-RNA action (since the S-217622 mol. can be considered as a uridine analog). Moreover, the idealistic drug-likeness and pharmacokinetic characteristics of S-217622 make it ready for pharmaceutical formulation with the expected very good clin. behavior as a drug for the infections caused by coronaviruses, e.g., COVID-19. To cut it short, the current critical findings of this extension work significantly potentiate and extend the S-217622 (previous in vitro/in vivo (preclin.) results since they showed that the striking inhibitory activities of this novel anti-SARS-CoV-2 agent on the M<sup>pro</sup> could be extended to other replication enzymes like RdRp and ExoN, unveiling the possible universal use of the compound against the next versions of the virus (i.e., disclosing the nonspecific anticonviral properties of this compound against almost any coronavirus strain), e.g., SARS-CoV-2, and encouraging us to rapidly start the compound's vast clin. anti-COVID-19 evaluations.



- Anti-M<sup>pro</sup> EC<sub>50</sub> (inhibitory work) = 0.17 μM
- Anti-RdRp EC<sub>50</sub> (inhibitory work) = 0.17 μM
- Anti-ExoN EC<sub>50</sub> (inhibitory work) = 0.27 μM
- Anti-SARS-CoV-2 EC<sub>50</sub> (inhibitory work) = 0.20-0.29 μM
- Anti-SARS-CoV-1 EC<sub>50</sub> (inhibitory work) = 0.21 μM
- Anti-MERS-CoV EC<sub>50</sub> (inhibitory work) = 1.40 μM
- Anti-HCoV-229E EC<sub>50</sub> (inhibitory work) = 0.90 μM
- Anti-HCoV-OC43 EC<sub>50</sub> (inhibitory work) = 0.874 μM

相互にリンク



# デモンストレーション

インフルエンザウイルスに対する生物活性情報を文献から検索する

Antiviral agents キーワードと組み合わせた検索

AND Disease Influenza

- Authors
- Publication Name
- Organization
- Title
- Abstract/Keywords
- Concept
- Substances
- Bioactivity Data NEW**
- Publication Year
- Document Identifier
- Patent Identifier
- Publisher

Search CAS Lexicon: Build powerful searches using CAS concepts, chemical classes, and taxonomy.

Search CAS Sequences: Query BLAST, CDR, and Motif algorithms for nucleotide and protein based sequences.

検索対象: Disease

View All Search History



# CAS Analytical Methods

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## CAS Analytical Methods

多岐にわたる分野の分析手法を効率的に検索

収録分野：

- 薬理学、HPLC 分析、食品分析、天然物単離分析、水分析など

収録内容：

- 測定機器、手順、バリデーションデータを含む詳細な分析情報

CAS が保有する文献コレクションから、  
分析の情報を抽出し、項目ごとに整理してデータベース化



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# CAS Analytical Methods

## 収録範囲

項目	内容
収録源	CAS SciFinder に収録の雑誌論文 例: Journal of Natural Medicines, Journal of Chromatography A, B, Journal of Pharmaceutical and Biomedical Analysis, Talanta, Analytica Chimica Acta
収録分野	医薬、農学、化学を中心とした科学分野
レコード構成	分析手法単位
収録期間	2000 年～

# CAS Analytical Methods

## レコード例

タイトル
物質情報
分析カテゴリー 分析手法名
使用機器、条件
分析手順
バリデーション (妥当性の検証結果)
収録源 (雑誌名、著者名、 出典のタイトル、抄録など)

### Analysis of $\beta$ -Carotene in Blood serum by Extraction

CAS Method Number: 2-114-CAS-43070

Method Category: Biomolecule Isolation Assay

Technique: Tandem mass spectrometry; Supercritical fluid chromatography; Extraction

Analyte	Matrix	Material	Reagent	Biological Reagent
Cryptoxanthin Zeaxanthin Lutein A $\beta$ -Carotene $\alpha$ -Carotene View All	Blood serum	Column (inner diameter: 250 mm x 4.6 mm, particle size: 5 $\mu$ m)		

**Equipment Used**  
SFC instrument: Waters, Milford, MA, USA  
MS instrument: Xevo TQ, Waters

**Conditions**  
**Instrument**  
Modifier: methanol with 0.1% (w/v) ammonium formate; back-pressure: 10 MPa; column temperature: 35 °C; flow rate: 3 mL/min  
polarity: positive; capillary voltage: 2.5 kV; cone voltage: 30 V; collision energy: 15 V; desolvation temperature: 600 °C; desolvation gas: 800 L/h; cone gas: 60 L/h

**Instructions**  
**Collection of serum samples**  
1. Collect serum samples from subjects.  
2. Purify low-density lipoprotein (LDL) from serum.  
**Process of extraction of carotenoids**  
1. Extract the carotenoids from the collected serum by using the following procedure.  
2. Add 0.1 mL of water, 0.2 mL of ethanol (including 10 ng/mL echinenone as an internal standard) and 1 mL of heptane with 5 mg/mL diethylhydroxytoluene to 0.1 mL of the serum and LDL (2.5 mg protein/mL) samples.  
3. Subsequently, allow the heptane layer to dry using nitrogen.  
4. Dissolve the residue in hexane and subsequently subject to SFC/MS/MS.  
**Supercritical fluid chromatography (SFC)/MS/MS**  
1. Analyze the sample/standard using SFC/MS/MS.  
2. Use Merck Purosphere RP-18e column maintained at 35 °C for analysis.  
3. Use methanol as modifier with 0.1% (w/v) ammonium formate 10 - 25% for 15 min, 25% for 2 min, 25 - 10% for 1 min and 10% for 2 min.  
4. Set the back-pressure as 10 MPa.  
5. Set the flow rate at 3 mL/min.  
6. Set the sample volume as 0.1 mL.  
7. Operate in electrospray ionization (ESI) mode.  
8. For MRM analysis, set the conditions as follows: polarity: positive; capillary voltage: 2.5 kV; cone voltage: 30 V; collision energy: 15 V; desolvation temperature: 600 °C; desolvation gas: 800 L/h and cone gas: 60 L/h.

# CAS Analytical Methods

レコード例

- タイトル
- 物質情報
- 分析カテゴリー  
分析手法名
- 使用機器、条件
- 分析手順
- バリデーション  
(妥当性の検証結果)
- 収録源  
(雑誌名、著者名、  
出典のタイトル、抄録など)

Validation	
Linearity Range	0.19 - 930 fmol, $\alpha$ -Carotene 0.47 - 930 fmol, $\beta$ -Carotene 0.18 - 910 fmol, $\beta$ -Cryptoxanthin 0.44 - 440 fmol, Lutein 0.44 - 440 fmol, Zeaxanthin
Limit of Detection	0.19 fmol, $\alpha$ -Carotene 0.093 fmol, $\beta$ -Carotene 0.091 fmol, $\beta$ -Cryptoxanthin 0.18 fmol, Lutein 0.18 fmol, Zeaxanthin
Retention Time	12.7 min, $\alpha$ -Carotene 14.0 min, $\beta$ -Carotene 8.6 min, $\beta$ -Cryptoxanthin 5.3 min, Lutein 5.3 min, Zeaxanthin 8.1 min, Epoxy- $\alpha$ -carotene 9.0 min, Epoxy- $\beta$ -carotene 6.0 min, Epoxy- $\beta$ -cryptoxanthin 3.8 min, Epoxy-lutein 4.1 min, Epoxy-Zeaxanthin
Concentration	79 nmol/L, $\alpha$ -Carotene 200 nmol/L, $\beta$ -Carotene 92 nmol/L, $\beta$ -Cryptoxanthin 490 nmol/L, Lutein 140 nmol/L, Zeaxanthin

Source

JOURNAL

Highly sensitive and rapid profiling method for carotenoids and their epoxidized products using supercritical fluid chromatography coupled with electrospray ionization-triple quadrupole mass spectrometry

Matsubara, Atsuki; Uchikata, Takato; Shinohara, Masakazu; Nishiumi, Shinji  
Journal of Bioscience and Bioengineering (2012), 113 (6), 782 - 787. Society for  
CODEN : JBBIF6 | ISSN : 13891723 | DOI : 10.1016/j.jbiosc.2012.01.017

View Abstract - Full Text - **View in CAS SciFinder**

CAS SciFinder との連携

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## デモンストレーション

蜂蜜 (honey) からグルコースを単離する分析手法を検索する

Explore Methods

Method Category

- Agricultural Applications / Analysis
- Bioassays
- Biomolecule Isolation**
- Environmental Analysis
- Food Analysis
- Fuels / Geology / Biofuels
- Historical Analysis / Dating
- Miscellaneous
- Organic Compound Analysis
- Organometallics / Inorganics
- Pharmacology / Toxicology
- Polymer Analysis
- Water Analysis

Method Subcategory

- Biomolecule Isolation Assay
- Natural Product Isolation Analysis**
- Protein Analysis

Include Keywords (Optional)

Search Methods

天然物の単離の手法を検索

カテゴリー検索

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# CAS FORMULUS

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## CAS Formulus

製剤・配合・成分情報を効率的に検索

重点分野：

- 医薬品、農薬、化粧品

一部収録分野：

- コーティング剤、日用品、食品、材料

内容収録：

- 配合の構成成分や機能、形状、各成分の価格情報や規制情報

文献および医薬添付文書から製剤・配合の情報を抽出し、  
項目ごとに整理してデータベース化



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# CAS Formulus

**Ingredients**

CAS RN: 33069-62-4

**Paclitaxel**

Key Physical Properties	Value
Molecular Weight	853.91
Melting Point (Experimental)	213-216 °C

Commonly Used As: Antitumor agents; Antiproliferative Coating materials...

Commonly Formulated With | Regulatory Information

**Formulations**

Herceptin-Functionalized Paclitaxel Nanocrystals: Drug Delivery or Anticancer--Controlled Release Drug Delivery Systems

Location: Article page 2, 4, Table 1

Purpose: Antitumor agents, Drug delivery systems

Target: Drugs, cancer cell growth

Physical Form: Nanocrystals

Component	Function	Amount Reported
Paclitaxel	Antitumor agents	20 mg
Trastuzumab	Antitumor agents	0.25 mg/mL

**成分情報へのリンク**

**配合情報へのリンク**

**CAS SciFinder との連携**

## 成分検索

- 物質名や機能性のキーワードから検索
- 物性、配合中の用途、配合情報へのリンク
- CAS SciFinder の物質詳細へのリンク

## 配合検索

- 配合成分や用途、ターゲット等から検索
- 成分や機能など配合の詳細、成分情報へのリンク
- CAS SciFinder の出典文献へのリンク

# デモンストレーション

抗がん性 (anticancer) の機能を持つ成分を検索し、その配合情報を検索する

**Good Afternoon**

Formulations Ingredients

Anticancer **抗がん性を持った成分を検索**

**Formulation Designer**  
Design custom formulation templates based on selections and ingredients

**Advanced Search**  
Search Formulations using criteria like ingredients, targets, and more.